Gravitational Corrections to the Energy-Levels of a Hydrogen Atom*

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The first order perturbations of the energy levels of a hydrogen atom in central internal gravitational field are investigated. The internal gravitational field is produced by the mass of the atomic nucleus. The energy shifts are calculated for the relativistic $1S$, $2S$, $2P$, $3S$, $3P$, $3D$, $4S$ and $4P$ levels with Schwarzschild metric. The calculated results show that the gravitational corrections are sensitive to the total angular momentum quantum number.

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I. INTRODUCTION

The study of gravitational fields interacting with spinor fields constitutes an important element in constructing a theory that combines quantum physics and gravity. For this reason, the investigation of the behavior of relativistic particles in this context is of considerable interest. It has been known that the energy levels of an atom placed in an external gravitational field will be shifted as a result of the interaction of the atom with space-time curvature see Refs. [1, 2, 3, 4] for examples. And the geometric and topological effects lead to shifts in the energy levels of a hydrogen atom are considered in Ref. [5].

Recently, there has been a dramatic increase in the accuracy of experiments that measure the transition frequencies in hydrogen. The most accurately measured transition is the $1S - 2S$ frequency in hydrogen; it has been measured with a relative uncertainty of 25 Hz ($\triangle f/f_0 = 1.0 \times 10^{-14}, f_0 = 2466$ THz) [6, 7], an order of magnitude larger than the natural linewidth of 1.3 Hz natural width of the $2S$ level [8, 9]. Indeed, it is likely that transitions in hydrogen will eventually be measured with an uncertainty below 1 Hz [10]. Though that accuracy can not explore the gravitational effect produced by the hydrogen atom nucleus, with the progress of experiments we can detect the gravitational effect.

In this paper we investigate another previously neglected gravitational effect of the energy-level shifts of a hydrogen atom. This is to give some explicit values for energy-level shifts of a hydrogen atom by the general relativistic effect with Schwarzschild metric. And the difference with Refs. [1, 2, 3, 4, 5] is that the gravitational field in this paper is not a external field but produced by the mass of hydrogen atom nucleus. To our knowledge no one has given explicit values for energy-level shifts of a hydrogen atom with gravitational corrections. Although the effect is very small, but it also has the physical significance as a test of general relativity at the quantum level.

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This paper is organized as follows: In Sec. II we review the formalism of the generally covariant Dirac equation in curved space-time. In Sec. III we give the tetrad and spinor connections with Schwarzschild metric. The gravitational perturbation of relativistic $1S$ level is calculated in Sec. IV. The summary and discussion are given in Sec. V.

II. GENERALLY COVARIANT DIRAC EQUATION IN CURVED SPACE-TIME

To write the generally covariant Dirac equation in curved space-time with metric $g_{\mu\nu}$, one first introduces the spinor affine connections $\omega_\mu = \frac{1}{2}\omega_\mu^{ab} I_{ab}$, where I_{ab} are the generators of $SO(4)$ group, whose spinor representation is

$$I_{ab} = \frac{1}{4}(\gamma_a\gamma_b - \gamma_b\gamma_a). \tag{1}$$

Here γ_a are the Dirac-Pauli matrices with the following relation

$$\gamma_a\gamma_b + \gamma_b\gamma_a = 2\eta_{ab}, \tag{2}$$

and

$$\gamma_0^\dagger = -\gamma_0, \quad \gamma_i^\dagger = \gamma_i \qquad (i = 1,2,3), \tag{3}$$

$$\gamma_0 = i\beta, \qquad \gamma_i = -i\beta\alpha_i. \tag{4}$$

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{5}$$

where I is the 2×2 identity matrix, $\eta^{ab} = \eta_{ab} = \mathrm{diag}(-1,1,1,1)$ is the Minkowski metric tensor, and σ_i are the standard Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{6}$$

ω_μ^{ab} is defined by the vanish of the generalized covariant derivative [11, 12] of the tetrad (or vierbein) field [13] $e^{(a)}{}_\mu(x)$

$$\begin{aligned} D_\mu e^{(a)}{}_\nu &= \partial_\mu e^{(a)}{}_\nu - \Gamma^\lambda_{\mu\nu} e^{(a)}{}_\lambda - \eta_{bc}\omega_\mu^{ab} e^{(c)}{}_\nu \\ &= \nabla_\mu e^{(a)}{}_\nu - \eta_{bc}\omega_\mu^{ab} e^{(c)}{}_\nu \equiv 0, \end{aligned} \tag{7}$$

where the tetrad field $e^{(a)}{}_\mu(x)$ and it's inverse $e_{(a)}{}^\mu(x)$ satisfy the following equations

$$g_{\mu\nu}(x) = \eta_{ab} e^{(a)}{}_\mu(x) e^{(b)}{}_\nu(x), \tag{8}$$

$$e^{(a)}{}_\mu(x) e_{(b)}{}^\mu(x) = \delta^a_b, \qquad (\mu,\nu,a,b = 0,1,2,3) \tag{9}$$

μ,ν are the space-time indices lowered with the metric $g_{\mu\nu}$, and a,b are the Lorentz group indices lowered with η_{ab}.

One also needs to introduce generalized Dirac-Pauli matrices $\Gamma_\mu(x) = e^{(a)}{}_\mu(x)\gamma_a$, which satisfy the equation [2]

$$\Gamma_\mu(x)\Gamma_\nu(x) + \Gamma_\nu(x)\Gamma_\mu(x) = 2g_{\mu\nu}(x). \tag{10}$$

The covariant derivative acting on a spinor field ψ is then

$$D_\mu\psi = \partial_\mu\psi - \omega_\mu\psi, \tag{11}$$

and the generally covariant form of the Dirac equation[4] in pure gravitational field is

$$\Gamma^\mu(x) D_\mu\psi(x) + \frac{mc}{\hbar}\psi(x) = 0, \tag{12}$$

where $\Gamma^\mu(x) = g^{\mu\nu}\Gamma_\nu(x)$, m is the mass of spinor particles.

For an electron near the atomic nucleus one needs to consider the effect of the electromagnetic vector potential A_μ, here A_μ satisfy the Maxwell equations [2, 14]

$$g^{\lambda\sigma}\nabla_\lambda\nabla_\sigma A_\mu - R_\mu{}^\nu A_\nu = -4\pi J_\mu, \tag{13}$$

where J_μ is the current vector. So the covariant derivative acting on a spinor field should be rewritten as

$$D_\mu\psi = (\partial_\mu - \omega_\mu - iqA_\mu)\psi. \tag{14}$$

Then the generally covariant form of the Dirac equation in gravitational and electromagnetic fields is

$$\Gamma^\mu(\partial_\mu - \omega_\mu - iqA_\mu)\psi(x) + \frac{mc}{\hbar}\psi(x) = 0. \tag{15}$$

III. SPINOR CONNECTIONS IN THE SCHWARZSCHILD SPACE-TIME

In what follows, we will calculate the spinor connections in a Schwarzschild spacetime. The line element corresponding to the spacetime is given by

$$\begin{aligned} ds^2 &= -g_{\mu\nu}dx^\mu dx^\nu \\ &= c^2\left(1 - \frac{R_s}{r}\right)dt^2 - \frac{1}{1-\frac{R_s}{r}}dr^2 - r^2 d\theta^2 - r^2\sin^2\theta d\phi^2, \end{aligned} \tag{16}$$

where $R_s = 2GM/r$. With the time gauge conditions [15, 16] $e^{(0)}{}_i = 0$ and $e_{(i)}{}^0 = 0$, the tetrad field $e^{(a)}{}_\mu$ is given as follows:

$$e^{(a)}{}_\mu = \begin{pmatrix} \sqrt{1-\frac{R_s}{r}} & 0 & 0 & 0 \\ 0 & \frac{\sin\theta\cos\phi}{\sqrt{1-\frac{R_s}{r}}} & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ 0 & \frac{\sin\theta\sin\phi}{\sqrt{1-\frac{R_s}{r}}} & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ 0 & \frac{\cos\theta}{\sqrt{1-\frac{R_s}{r}}} & -r\sin\theta & 0 \end{pmatrix}. \tag{17}$$

Taking the approximation $\sqrt{1-\frac{R_s}{r}} \cong 1 - \frac{R_s}{2r}$, we have

$$e^{(a)}{}_\mu = \begin{pmatrix} 1-\frac{R_s}{2r} & 0 & 0 & 0 \\ 0 & \frac{\sin\theta\cos\phi}{1-\frac{R_s}{2r}} & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ 0 & \frac{\sin\theta\sin\phi}{1-\frac{R_s}{2r}} & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ 0 & \frac{\cos\theta}{1-\frac{R_s}{2r}} & -r\sin\theta & 0 \end{pmatrix}. \tag{18}$$

From Eq. (7), it follows

$$\omega_\mu^{ab} = (\nabla_\mu e^{(a)}{}_\nu)e^{(b)}{}_\lambda g^{\lambda\nu}, \tag{19}$$

and

$$\omega_\mu = \frac{1}{2}\omega_\mu^{ab}I_{ab} = \frac{1}{2}I_{ab}(\nabla_\mu e^{(a)}{}_\nu)e^{(b)}{}_\lambda g^{\lambda\nu} \approx \frac{1}{2}I_{ab}(-\Gamma^\rho_{\mu\nu})e^{(a)}{}_\rho e^{(b)}{}_\lambda g^{\lambda\nu}. \tag{20}$$

Thus using Eqs. (16), (18), (19)and (20), we obtain the explicit expressions of the nonzero components of spinor connections

$$\omega_0 = \begin{pmatrix} 0 & 0 & -\frac{R_s\cos\theta}{4r^2} & -\frac{R_s\sin\theta\ e^{-i\phi}}{4r^2} \\ 0 & 0 & -\frac{R_s\sin\theta\ e^{i\phi}}{4r^2} & \frac{R_s\cos\theta}{4r^2} \\ -\frac{R_s\cos\theta}{4r^2} & -\frac{R_s\sin\theta e^{-i\phi}}{4r^2} & 0 & 0 \\ -\frac{R_s\sin\theta\ e^{i\phi}}{4r^2} & \frac{R_s\cos\theta}{4r^2} & 0 & 0 \end{pmatrix}, \tag{21}$$

$$\omega_2 = \begin{pmatrix} 0 & \frac{(r-R_s)e^{-i\phi}}{2r-R_s} & 0 & 0 \\ -\frac{(r-R_s)e^{i\phi}}{2r-R_s} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{(r-R_s)e^{-i\phi}}{2r-R_s} \\ 0 & 0 & -\frac{(r-R_s)e^{i\phi}}{2r-R_s} & 0 \end{pmatrix}, \tag{22}$$

$$\omega_3 = \begin{pmatrix} \frac{iC_1}{8r-4R_s} & \frac{R_s\sin 2\theta\ ie^{-i\phi}}{8r-4R_s} & 0 & 0 \\ \frac{iR_s\sin 2\theta\ e^{i\phi}}{8r-4R_s} & -\frac{iC_1}{8r-4R_s} & 0 & 0 \\ 0 & 0 & \frac{iC_1}{8r-4R_s} & \frac{R_s\sin 2\theta\ ie^{-i\phi}}{8r-4R_s} \\ 0 & 0 & \frac{iR_s\sin 2\theta\ e^{i\phi}}{8r-4R_s} & -\frac{iC_1}{8r-4R_s} \end{pmatrix}, \tag{23}$$

where

$$C_1 = 4r - 3R_s + R_s\cos(2\theta). \tag{24}$$

IV. GRAVITATIONAL PERTURBATION OF THE RELATIVISTIC HYDROGEN ATOM: THE $1S_{1/2}$ STATES

From Eq. (15) the corresponding Hamiltonian in curved space-time follows

$$H = -i\hbar c\Gamma_0\Gamma^i(\partial_i - \omega_i - iqA_i) + i\hbar c(\omega_0 + iqA_0) - imc^2\Gamma_0. \tag{25}$$

The Dirac Hamiltonian in flat space is

$$H_0 = -i\hbar c\gamma_0\gamma^i(\partial_i - iqA_i^{'}) - \hbar cqA_0^{'} - imc^2\gamma_0, \tag{26}$$

where $A_\mu^{'}$ are the electromagnetic vector potentials in flat spacetime. Here we can take the approximation $A_i \cong A_i^{'} = 0$ and $A_0 \cong A_0^{'} = -er^{-1}$, the detailed discussions of this problem is contained in Ref. [2]. So the Hamiltonian of the gravitational perturbation is given by

$$\begin{aligned} H_I &= H - H_0 \\ &= -i\hbar c\Gamma_0\Gamma^i(\partial_i - \omega_i) + i\hbar c\omega_0 - im_ec^2\Gamma_0 \\ &\quad + i\hbar c\gamma_0\gamma^i\partial_i + im_ec^2\gamma_0. \end{aligned} \tag{27}$$

The exact solutions of the Dirac equation for a hydrogen atom in flat space-time serve as the basis for perturbation theory. The energy eigenvalues of a hydrogen atom are

$$E_{n\kappa} = m_ec^2\sqrt{1 + \left(\frac{\zeta}{n - |\kappa| + s}\right)^2}, \tag{28}$$

where $\zeta = Ze^2$, $s = \sqrt{\kappa^2 - \zeta^2}$, $n = 1, 2, \cdots$ is the principal quantum number.

The bound state functions of a hydrogen atom can be written in standard representation [17, 18] as

$$\psi = \psi_\kappa^M = \begin{pmatrix} g(r)\chi_\kappa^M \\ -if(r)\chi_{-\kappa}^M \end{pmatrix}, \tag{29}$$

here M is the eigenvalue of J_z, κ is the eigenvalue of $K = \beta(\vec{\sigma} \cdot \vec{L} + I)$, the functions $f(r)$, $g(r)$ and spinors χ_κ^M, $\chi_{-\kappa}^M$ are given by

$$\begin{aligned} f(r) &= \frac{2^{s-\frac{1}{2}}\lambda^{s+\frac{3}{2}}}{\Gamma(2s+1)}\sqrt{\frac{\Gamma(2s+n_r+1)}{n_r!\zeta K_c(\zeta K_c - \lambda\kappa)}}\sqrt{1 - \frac{W_c}{K_c}} r^{s-1} e^{-\lambda r} \\ &\left(\left(\kappa - \frac{\zeta K_c}{\lambda}\right)\mathrm{F}(-n_r, 2s+1, 2\lambda r) - n_r \mathrm{F}(-n_r+1, 2s+1, 2\lambda r)\right), \end{aligned} \tag{30}$$

$$\begin{aligned} g(r) &= -\frac{2^{s-\frac{1}{2}}\lambda^{s+\frac{3}{2}}}{\Gamma(2s+1)}\sqrt{\frac{\Gamma(2s+n_r+1)}{n_r!\zeta K_c(\zeta K_c - \lambda\kappa)}}\sqrt{1 - \frac{W_c}{K_c}} r^{s-1} e^{-\lambda r} \\ &\left(\left(\kappa - \frac{\zeta K_c}{\lambda}\right)\mathrm{F}(-n_r, 2s+1, 2\lambda r) + n_r \mathrm{F}(-n_r+1, 2s+1, 2\lambda r)\right), \end{aligned} \tag{31}$$

$$\chi_\kappa^M = C_{1/2} Y_l^{M-1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + C_{-1/2} Y_l^{M+1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{32}$$

$$\chi_{-\kappa}^M = -C_{1/2} Y_l^{M-1/2} \begin{pmatrix} \cos\theta \\ e^{i\phi}\sin\theta \end{pmatrix} - C_{-1/2} Y_l^{M+1/2} \begin{pmatrix} e^{-i\phi}\sin\theta \\ -\cos\theta \end{pmatrix}, \tag{33}$$

where $W_c = E_{n\kappa}/m_e c^2$, $K_c = m_e c^2/\hbar c$, $\lambda = \sqrt{m_e^2 c^4 - E_{n\kappa}^2}/\hbar c$, $C_{1/2}$ and $C_{-1/2}$ are the C-G coefficients.

For a hydrogen atom there are two $1S_{1/2}(n = 1, l = 0, J = 1/2, \kappa = -1)$ states, which correspond to $M = \pm 1/2$. The states can be written as

$$\psi_1 = \begin{pmatrix} 0 \\ f(r) \\ ig(r)\sin\theta e^{-i\phi} \\ -ig(r)\cos\theta \end{pmatrix}, \tag{34}$$

and

$$\psi_2 = \begin{pmatrix} f(r) \\ 0 \\ ig(r)\cos\theta \\ ig(r)\sin\theta e^{i\phi} \end{pmatrix}, \tag{35}$$

where ψ_1 corresponds to $M = 1/2$ and ψ_2 to $M = -1/2$,

$$f(r) = \frac{2^{-\frac{3}{2}+s} e^{-r\lambda} r^{-1+s} \lambda^{\frac{1}{2}+s}\sqrt{K_c + W_c}\sqrt{K_c\zeta + \lambda}}{K_c\sqrt{\pi\zeta\Gamma(1+2s)}}, \tag{36}$$

$$g(r) = \frac{2^{-\frac{3}{2}+s} e^{-r\lambda} r^{-1+s} \lambda^{\frac{1}{2}+s}\sqrt{K_c - W_c}\sqrt{K_c\zeta + \lambda}}{K_c\sqrt{\pi\zeta\Gamma(1+2s)}}, \tag{37}$$

$\Gamma(1+2s)$ is the Γ function. The gravitational perturbation matrix elements are

$$\langle H_I \rangle_{ab} \equiv (\psi_a, H_I \psi_b), \tag{38}$$

where the subscripts a, b take on the values $1, 2$. Because we take the gravitational field metric as the Schwarzschild metric, so we need to confirm the range of the integration. Here it is taken from R_n to ∞, $R_n \cong 1.3 \times 10^{-15}$ m is the atomic nucleus radius. With the computer algebra system Mathematica, we obtain the following results for those perturbation matrix elements

$$\langle H_I \rangle_{ab} = -\frac{\delta_{ab}}{K_c^2 R_n \zeta \Gamma(1+2s)} 2^{-1+2s} c R_s \lambda (R_n \lambda)^{2s} (K_c \zeta + \lambda) \left(cm R_n W_c \mathrm{E}_{1-2s}(2R_n\lambda) + \sqrt{K_c^2 - W_c^2}\hbar \mathrm{E}_{2-2s}(2R_n\lambda) \right), \tag{39}$$

where $\mathrm{E}_n(z) = \int_1^\infty e^{zt}/t^n dt$ is the exponential integral function. Using the equation [2]

$$\det[(\psi_a, H_I\psi_b) - E_i^{\,1}\delta_{ab}] = 0, \tag{40}$$

from the usual perturbation theory of a degenerate energy eigenvalue, it follows that both of the degenerate $1S_{1/2}$ levels are shifted by the same perturbation:

$$E^1(1S_{1/2}) = -\frac{1}{K_c^2 R_n \zeta \Gamma(1+2s)} 2^{-1+2s} c R_s \lambda (R_n \lambda)^{2s} (K_c \zeta + \lambda) \left(cm R_n W_c \mathrm{E}_{1-2s}(2R_n\lambda) + \sqrt{K_c^2 - W_c^2}\hbar \mathrm{E}_{2-2s}(2R_n\lambda) \right). \tag{41}$$

Substituting the constant values in Table 1 into Eq. (41), we get

$$E^1(1S_{1/2}) = -1.19956 \times 10^{-38} \text{ ev}. \tag{42}$$

TABLE 1. The constants table [19]

Quantity	Symbol	Value	Units
electron charge magnitude	e	$1.60217653 \times 10^{-19}$	C
speed of light in vacuum	c	$2.99792458 \times 10^{-8}$	m s^{-1}
electron mass	m_e	$9.91093826 \times 10^{-31}$	kg
Planck constant, reduced	$\hbar$	$1.05457168 \times 10^{-34}$	J s
permittivity of free space	ϵ_0	$8.854187817 \times 10^{-12}$	s^4 A^2 kg^{-1} m^{-3}
proton mass	M_p	$1.67262171 \times 10^{-27}$	kg
gravitation constant	G	6.6742×10^{-11}	m^3 kg^{-1}s^{-2}

V. SUMMARY AND DISCUSSION

In a similar calculation as the $1S_{1/2}$ state, we find that all the relativistic $1S$, $2S$, $2P$, $3S$, $3P$, $3D$, $4S$ and $4P$ energy levels are respectively shifted as the same amount listed in Table 2. This means that the first order gravitational perturbations can partly remove the degeneracy of the hydrogen atom states. Although the effect is very small, but form Table 2 we find that the quantity of corrections of the energy levels with same principal quantum number n and total angular momentum quantum number J, like $2S_{1/2}$ and $2P_{1/2}$, $3S_{1/2}$ and $3P_{1/2}$, $3P_{3/2}$ and $3D_{3/2}$, are very closely. But for the levels with same principal quantum number and different total angular momentum quantum number, like $3S_{1/2}$ and $3P_{3/2}$, their corrections have obvious difference. Those calculations show that the gravitational corrections are sensitive to the total angular momentum quantum number. It is a very important feature of the interaction between gravitational fields and spinor fields. With this feature we can find the gravitational effect in other system, and make a test of general relativity at the quantum level.

TABLE 2. The energy-level shifts

State	The energy-level shift (Unit: ev)
$1S_{1/2}$	-1.19956 $\times 10^{-38}$
$2S_{1/2}$	-8.99637 $\times 10^{-39}$
$2P_{1/2}$	-8.99562 $\times 10^{-39}$
$2P_{3/2}$	-2.99862 $\times 10^{-39}$
$3S_{1/2}$	-6.66389 $\times 10^{-39}$
$3P_{1/2}$	-6.66353 $\times 10^{-39}$
$3P_{3/2}$	-2.66544 $\times 10^{-39}$
$3D_{3/2}$	-2.66538 $\times 10^{-39}$
$4S_{1/2}$	-5.24777 $\times 10^{-39}$
$4P_{1/2}$	-5.24756 $\times 10^{-39}$

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